Stochastic simulation of thermoemission from surfaces of dusty grains.

A.L. Bondareva, V.D. Levchenko, G.I. Zmievskaya

Keldysh Institute of applied mathematics RAS, 125047 Miusskaya sq., 4 Moscow Russia, bal@spp.keldysh.ru

Abstract. The thermoemission from dusty grains surfaces is necessary to take into account when processes in dusty plasma are simulated. The thermoemission of electrons can change temperature of electron part of plasma, typical electron velocity and others plasma properties. The kinetic distribution functions of secondary electrons from velocity and distance from dusty grain are calculated.

The paper deals with stochastic simulation of plasma-surface interaction processes such as thermoemission and secondary emission of electrons, emission of adatoms, elastic and inelastic reflecions of plasma particles from dusty grains surfaces, ions and electrons penetrations into dusty grains. All these processes not only change dusty grains surfaces behaviour but also promote to plasma pollution and change plasma properties. Study of these processes is necessary for microelectronics, nanotechnology, cosmophysics and gas discharges.
Special attention is paid to thermoemission. The model is supplement with selfconsistent three dimensional kinetic code of processes in dusty plasma [1-4]. Note, that model presented in this paper has not self-consistency, dusty charge, size, temperature and electrostatic potential are supposed constants. This work will be introduced into main object-oriented 3D3V kinetic dusty plasma C++ code SUR-Dust [1-4] as its part. Change dusty charge, size, temperature and electrostatic potential also as change of plasma parameters (such as temperatures and densities of plasma components and others) take place only in main code and only main code is selfconsistent [1-4]. Simulation of processes on dusty grains surface is based on kinetic theory, Brownian motion model and stochastic analogues methods. The Leontovich equation is associated with the brownian motion model and Kramers problem. Emission under the influence of ions and electrons is described in terms of jump like Markov processes. Thermoemission and emission of adatoms from surface are simulated by diffusion Markov processes [5].The equation for thermoemission of electrons can be presented as follows:

$$\frac{\partial f}{\partial t} + v_r \frac{\partial f}{\partial r} + \frac{e}{m_e}\frac{\partial U}{\partial r}\frac{\partial f}{\partial v_r} = \gamma \frac{\partial(\vec{v} f)}{\partial \vec{v}} + \frac{\gamma T}{m_e}\frac{\partial^2 f}{\partial \vec{v}^2} \tag{1}$$

$$U(r) = \begin{cases} \left(\dfrac{Q}{R_d/a} - A_{out}\right)\left(1 + \alpha \cos\dfrac{2\pi r}{a}\right), & r/a \le R_d/a - 1 \\ 1.58\dfrac{\dfrac{Q}{R_d/a} - A_{out}}{1 + \exp\left(\dfrac{3(r - R_d)}{a}\right)}, & R_d/a - 1 \le r/a \le R_d/a + 2 \\ \dfrac{Q}{r/a}, & r/a \ge R_d/a + 2 \end{cases} \tag{2}$$

here r is distance from centre of dusty grain, $\vec{v}$, v_r are electron velocity and its radial component, f is distribution function of electrons from velocities and coordinates, e, m_e are charge and mass of electrons, R_d is radius of dusty grain, $\gamma = \gamma(r)$ is damping parameter, $\gamma = const \neq 0$ if $r \le R_d$ and $\gamma = 0$ if $r = R_d$, R_d, Q are radius and charge of dusty particle, a is lattice parameter, A_{out} is work function for material of dusty grain. All parameters are presented in dimensionless quantities. In physical quantities $R_d = 100\ a$, $a = 3.5$ Å, $A_{out} = 12$ eV. The potential $U(r)$ in eV is presented in following figure.

CP762, *Rarefied Gas Dynamics: 24th International Symposium,* edited by M. Capitelli

Report Documentation Page

Form Approved
OMB No. 0704-0188

1. REPORT DATE	2. REPORT TYPE	3. DATES COVERED
13 JUL 2005	**N/A**	**-**

4. TITLE AND SUBTITLE **Stochastic simulation of thermoemission from surfaces of dusty grains**	5a. CONTRACT NUMBER 5b. GRANT NUMBER 5c. PROGRAM ELEMENT NUMBER
6. AUTHOR(S)	5d. PROJECT NUMBER 5e. TASK NUMBER 5f. WORK UNIT NUMBER
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) **Keldysh Institute of applied mathematics RAS, 125047 Miusskaya sq., 4 Moscow Russia**	8. PERFORMING ORGANIZATION REPORT NUMBER
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)	10. SPONSOR/MONITOR’S ACRONYM(S) 11. SPONSOR/MONITOR’S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release, distribution unlimited

13. SUPPLEMENTARY NOTES
See also ADM001792, International Symposium on Rarefied Gas Dynamics (24th) Held in Monopoli (Bari), Italy on 10-16 July 2004. , The original document contains color images.

14. ABSTRACT

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT **unclassified**	b. ABSTRACT **unclassified**	c. THIS PAGE **unclassified**	**UU**	**4**	

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std Z39-18

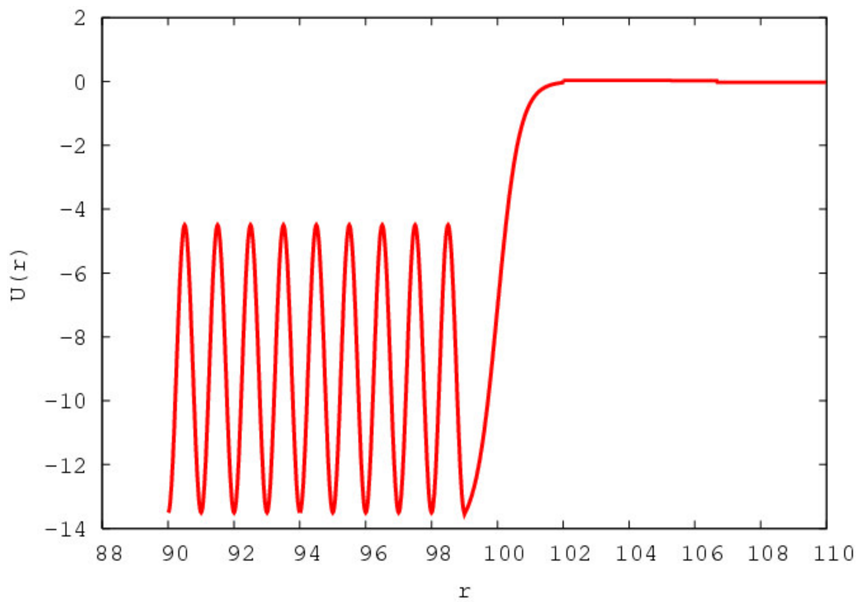

FIGURE 1. The U(r) inside ($r \leq R_d$) and outside ($r > R_d$) of dusty grain is shown, here r is distance from centre of dusty grain measured in lattice parameters a, R_d=100a.

The solving of receiving kinetic equation for thermoemission the splitting method is used. The system of kinetic equation is solved. The determined and stochastic part are separated. The solution of Leontovich equation for $f(\vec{v}, \vec{r}, t)$ is changed solution of equations systems:

$$\begin{cases} \dfrac{\partial f_1}{\partial t} + v_r \dfrac{\partial f_1}{\partial t} + \dfrac{e}{m_e} \dfrac{\partial U}{\partial r} \dfrac{\partial f_1}{\partial v_r} = 0 \\ f_1(r, v_r, t = t_0) = f(r, v_r, t = t_0) \end{cases} \tag{3}$$

and

$$\begin{cases} \dfrac{\partial f_2}{\partial t} = \gamma \dfrac{\partial(\vec{v} f)}{\partial \vec{v}} + \dfrac{\gamma T}{m_e} \dfrac{\partial^2 f}{\partial v^2} \\ f_2(r, v_r, t = t_0) = f_1(r, v_r, t = t_0 + \Delta t) \\ f(r, v_r, t = t_0 + \Delta t) = f_2(r, v_r, t = t_0 + \Delta t) \end{cases} \tag{4}$$

The first equation (3) is solved using centred explicit second order leap-frog scheme, and the second equation (4) containing stochastic part has been replaced to suitable stochastic analogue and solved using modified Artem'ev method [6].

RESULTS AND DISCUSSION

The kinetic approach lets to receive not only macrocharacteristic of particles leaving of dusty grains surfaces, but also these distribution functions from space coordinates and velocities. As a result of numerical experiments authors present distribution function from velocities $f(v_r)$. The emitted particles from dusty grains change the plasma parameters. Hence them distribution functions are necessary for development of completely

selfconsistent kinetic model of dusty plasma and numerical 3D3V code for simulation the processes in dusty plasma.
The figure 2 shows the distribution functions $f(v_r)$ from radial component of velocities at finish moment of time. As can see, development some maximums of $f(v_r)$ is observed. Maximum conforming to electrons with small radial component of velocities (less than 6 thermal velocities) is more pronounced, it connects with big number of electrons with small energy. Maximum corresponding to electrons with high velocities becomes more outlined and part of secondary electrons with high velocity as well as typical velocity of electron increase when dusty grain temperature increase.

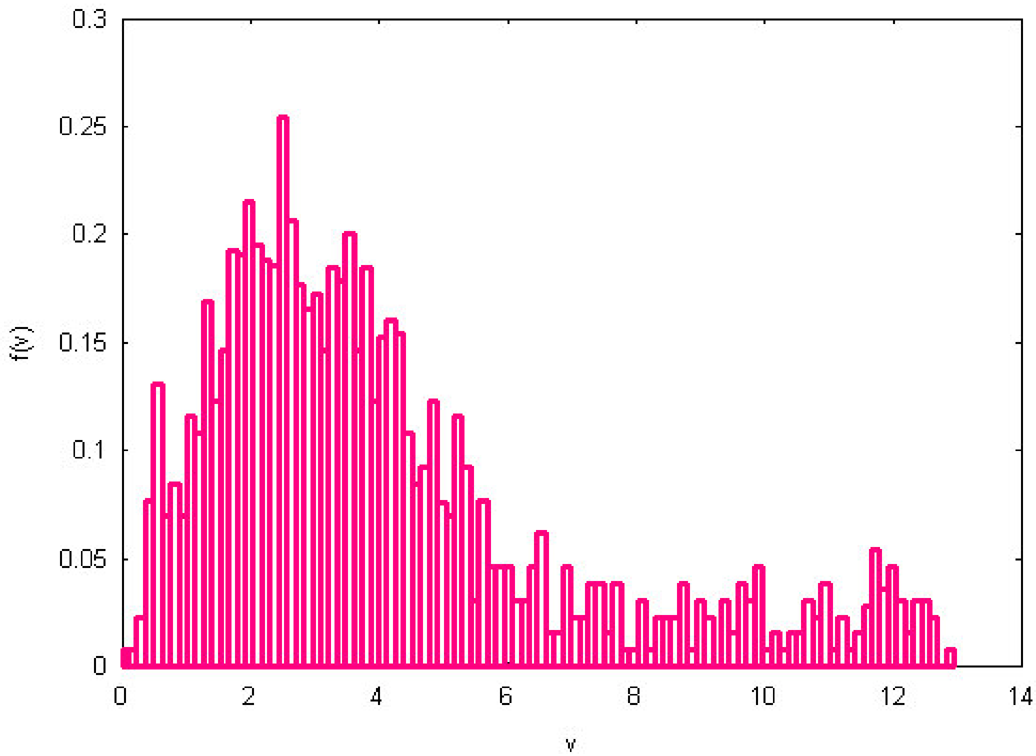

FIGURE 2. The distribution functions $f(v_r)$ from radial component of velocities is shown at finish of calculation. The temperature of dusty grain surface is 2.5 eV. We used 10^6 trajectories for received the distribution functions.

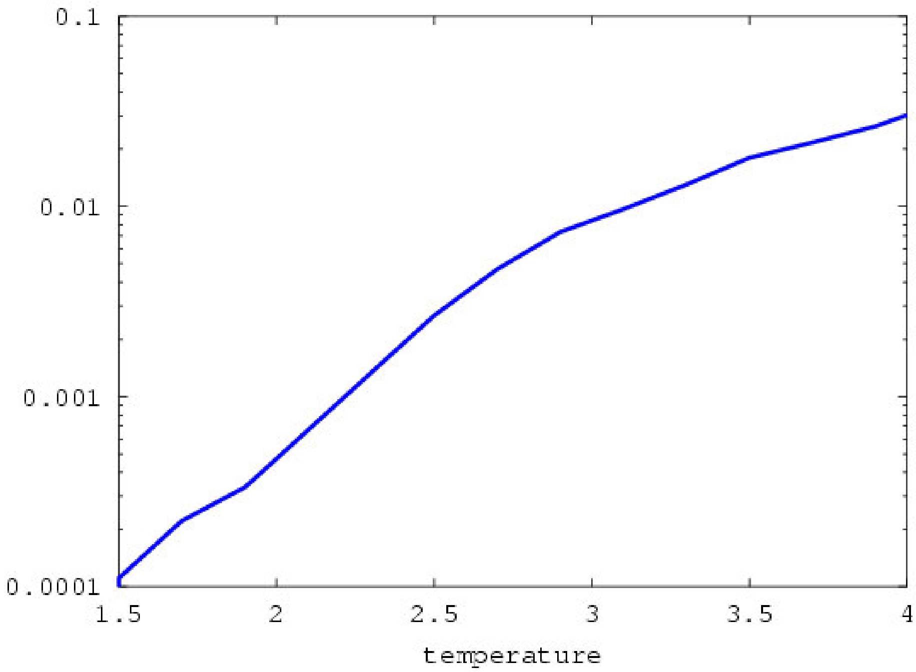

FIGURE 3. The logarithm of ratio of number of electrons left grain surface to total electron number is presented on this figure. The particle temperature is measured in eV and shown on abscissa axis.

The presented on fig. 3 dependence looks like law of Richardson-Deshman in low temperature region, the variances from Richardson-Deshman form in high temperature region concern non-stationarity of distribution functions $f(v_r)$ of electrons inside dusty grains. The process of change of dusty grains charge as a result of electrons thermoemission is necessary take into account if dusty grain surface temperature is more then 4 eV.

ACKNOWLEDGMENTS

The work is partially supported by Russian Science Support Foundation, RFBR grant 02-01-01004, the program "Nanoparticles and nanotechnology" by Department of Mathematical Sciences RAS 3.5 and scientific school 1388.2003.2.

REFERENCE

[1] V.D.Levchenko, L.V.Inkov, G.I.Zmievskaya.// 30th EPS Conf. CFPP St. Petersburg, Russia. v. ECA 27A p.O-1.6B, 1-4. (2003)

[2] V.D.Levchenko, L.V.Inkov, G.I.Zmievskaya, T.V. Levchenko //Poverkhnost' (The Surface). X-ray, synchrotron and neutron investigations, N 5, 2004, pp. 106-111 (in russ.)

[3] Levchenko V.D., Sigov Yu. S. //in book Dynamics of transport in plasmas and charged beams, ds.G.Maino and M.Ottaviani, World Sci.Publish.1996, p.55-69 ISBN:9810221541

[4] Zmievskaya G.I. // Plasma Phys Rep.V. 23, N 4, 1997, p. 45

[5] Yu. N. Devyatko, F.N. Markun//Materials of 16th International conference "Ion-Surface Interactions ISI-2003", Vol. 1, 2003, pp. 466-468

[6] Artemiev S.S., Averina T.A. Numerical analysis of systems of ordinary and stochastic differential equations.-Utrecht, The Netherlands, 1997, 176